Our research program is focused on the study of the structure and dynamics of disordered and partially ordered condensed matter at the atomic and molecular levels with a special emphasis on phase transitions. The purpose of these investigations is to discover the basic laws of physics governing the behaviour of these systems, which represent the link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems, on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research program is devoted to the development of new experimental methods and techniques in the field of magnetic resonance, magnetic resonance imaging, fluorescence microspectroscopy, scanning tunnelling, electronic and atomic force microscopy, as well as dielectric relaxation spectroscopy and dynamic specific-heat measurements.

The experimental techniques used are:
- One-(1D) and two-dimensional (2D) nuclear magnetic resonance (NMR) and relaxation, as well as quadrupole (NQR) resonance and relaxation,
- Multi-frequency NMR in superconducting magnets of 2 T, 6 T and 9 T, as well as the dispersion of the spin-lattice relaxation time $T_1$, via field cycling,
- Nuclear double resonance and quadrupole double resonance such as $^{17}$O–H and $^{14}$N–H,
- Fast field cycling NMR relaxometry,
- Frequency-dependent electron paramagnetic resonance (EPR) and 1D and 2D pulsed EPR and relaxation,
- MR imaging and micro-imaging,
- Measurement of the electronic transport properties,
- Magnetic measurements,
- Fluorescence microscopy and microspectroscopy,
- Linear and non-linear dielectric spectroscopy in the range $10^{-2}$ Hz to $10^9$ Hz,
- Electron microscopy and scanning tunnelling microscopy,
- Atomic force microscopy and force spectroscopy,
- Dynamic specific heat measurements.

The research program of the Department of Solid State Physics at the “Jožef Stefan” Institute is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the J. Stefan International Postgraduate School. In 2012, the research was performed within three research programs:
- Magnetic resonance and dielectric spectroscopy of smart new materials
- Physics of Soft Matter, Surfaces and Nanostructures
- Experimental Biophysics of Complex Systems

I. Research programme “Magnetic resonance and dielectric spectroscopy of smart new materials”

In 2012 the members of the program group published 55 original scientific papers in international peer-reviewed scientific journals. Several articles were published in high-impact journals (one article in Nature Photonics, one in Chemical Society Reviews and four articles in Phys. Rev. Letters). The investigations were focused on the following research fields.

Quasicrystals and complex metallic alloys

We have determined the anisotropic physical properties of decagonal quasicrystal d-Al-Co-Ni and demonstrated the anisotropy of the transport coefficients (electrical resistivity, thermoelectric...
The group has investigated important open issues in the electronic properties of quasicrystals and complex metallic alloys, quantum magnetism in low-dimensional spin systems, critical properties of nanostructures, physical properties of materials with giant electrocaloric and thermoelastic effects, new metallic materials for hydrogen storage and developed novel pharmaceutical and biological substances. The group has also developed a novel spectroscopic method utilizing polarized X-rays on the nanometric scale.

Figure 2: Characteristic temperature-dependent electrical resistivity and thermoelectric power of icosahedral quasicrystals, exhibiting a pseudogap in the electronic density of states at the Fermi energy.

Figure 3: Characteristic phase diagram of a one-dimensional quantum antiferromagnet around the critical field $B_{c1}$ contains three phases with different spin excitations: with magnons (gapped), with spinons (TLL) and intermediate quantum critical region.

Quantum magnetism

By means of NMR spin-lattice relaxation time, we have studied the spin dynamics as a function of the magnetic field in two quasi-one-dimensional quantum antiferromagnets: the anisotropic spin-chain system NiCl$_2$-4SO(NH$_2$)$_2$ and the spin-ladder system $(C_6H_9N)_2CuBr$_4$. We confirmed that the spin excitations in both systems evolve from magnons to spinons when crossing the critical field, in accordance with theoretical predictions. In the vicinity of the critical field, we showed that spin excitations are neither magnons nor spinons, while the spin dynamics scales in accordance with quantum criticality. We showed that the behaviour in both systems is equivalent, thus demonstrating the universality of quantum-critical behaviour. The work was published in Phys. Rev. Lett., see Figure 3.

Members of our department together with a group of international collaborators investigated the ground state of the geometrically frustrated system FeTe$_2$O$_3$Br, which is characterized by low-temperature multiferroicity. We have shown that the emergence of an incommensurate amplitude-modulated magnetic structure depends on the magnetic frustration that originates from the topology of this particular spin system. Surprisingly, the system is in fact characterized by magnetic chains, which are coupled by frustrated exchange interactions. The same group of authors investigated the stability of the incommensurate magnetic ordering at the lowest experimentally accessible temperatures using neutron diffraction measurements at 53 mK. Muon relaxation measurements have revealed that in spite of long-range ordering the spin dynamics does not freeze even in the limit of $T \to 0$ (Figure 4). The amplitude-modulated magnetic structures serve as a model system for the coexistence of long-range order and persistent spin dynamics.

A layered Kagome-like Cu$_3$(SeO$_3$)$_2$O$_3$Br compound was studied using neutron diffraction, bulk magnetization and magnetic susceptibility measurements. At $T_c \simeq 27.4$ K a transition into the long-range antiferromagnetic ordered phase occurred. The magnetic structure is composed of alternating ferrimagnetic ab layers, with the Cu$^{2+}$ ($S=1/2$) magnetic moments slightly canting away from the c axis. This magnetic structure was ascribed to the competition between ferro- and antiferro-magnetic interactions within the ab layers and additional weak antiferromagnetic interlayer interactions. When the magnetic field perpendicular to the layers exceeds $B_c \simeq 0.8$ T, a metamagnetic transition occurs, where every second layer flips (Figure 5). In combination with other techniques we were able to estimate the strength of individual Cu$^{2+}$-Cu exchange interactions.

Spectroscopy with polarized X-rays at the nanoscale

Near-edge X-ray absorption spectroscopy (NEXAFS) is an essential analytical tool in material science. Combining NEXAFS with scanning transmission X-ray microscopy (STXM) adds spatial resolution and the possibility to study individual nanostructures. In an article published in Nature Photonics, we described a full-field transmission X-ray microscope (TXM) that generates high-resolution, large-area NEXAFS data with a collection rate two orders of magnitude faster than is possible with STXM (Figure 6). We present image stacks and polarization-dependent NEXAFS spectra from individual anisotropic sodium and protonated titanate nanoribbons ((Na, H)TiNRs, HTINRs)). The combined NEXAFS-TXM technique has the advantage that one image stack visualizes...
a large number of nanostructures and therefore already contains statistical information. This new high-resolution NEXAFS-TXM technique opens the way to advanced nanoscale science studies.

Study of the critical properties of nanostructured materials and materials with large electrocaloric and thermomechanical effects

We showed that the refrigerant capacity of PLZT ceramics and ferroelectric polymer films exceed several times all previously known materials, including the magnetocaloric materials. By using high-resolution calorimetry we proved the existence of the phase transition line between the glassy and ferroelectric phase of relaxor ferroelectrics (Figure 7) and explained the anisotropy of criticality in these systems. We described the way to control the temperature profile of the thermomechanical response in liquid crystal elastomers via different physical parameters such as mechanical fields and the state of the order during the crosslinking procedure. We showed that highly confined liquid crystals exhibit a crossover in the dimensionality of the problem.

Relaxor polymers and ceramic materials

In collaboration with researchers from the Pennsylvania State University, USA, the electrically-induced behaviour was compared in a non-stretched and uniaxially stretched P(VDF-TrFE-CFE) terpolymer - a member of the relaxor polymer family that exhibits fast response speeds, giant electrostriction, high electric energy density, and a large electrocaloric effect. Substantial differences in the dielectric response, polarization, electrocaloric response, and induced electrostrictive strain of the non-stretched and stretched terpolymer were detected and explained. The results suggest that the electrically-induced properties of relaxor polymer films can be tailored by controlling the preparation conditions. In collaboration with researchers from Nanjing University, China, we have reported on the structural, thermal, and dielectric properties of relaxor P(VDF)-based terpolymer/copolymer blends on aluminum foil, i.e., the first relaxor polymer blends developed on a metal surface. The detected response has been explained by calculations that take into account the fact that two similar dynamic processes (relaxor dynamics in the crystalline regions and a glassy transition in the amorphous matrix) superimpose in the same temperature range (Figure 8).

The dielectric response of core-shell structured ceramic materials (composed of semiconducting grains separated by insulating grain boundaries) has been modelled in terms of an equivalent electric circuit with elements that describe distinctive contributions of grains and grain boundaries. By taking into account a proper temperature dependence of the individual elements of the circuit, the temperature- and frequency-dependent dispersive dielectric behaviour, typically observed in these materials, has been obtained. The modelling results have been applied to the experimentally detected dielectric response of CaCu3Ti4O12 thin films that exhibit, for a ceramic thin film, extremely high values of the dielectric constant. In addition, the influence of parasitic inductance and the resistance of the experimental setup on the measured dielectric response was calculated. A novel experimental setup has been installed in 2012 that enables a simultaneous detection of the electrical (four-point electrical conductivity) and thermoelectrical (thermoelectric voltage, the Seebeck coefficient) properties from room temperature up to 1000°C.

Hydrogen-storage metallic alloys

The crystal structure, bonding and magnetic changes upon hydrogenation of TiFe1-xNi2 alloys with different hydrogen and Ni contents were investigated (Figure 9). In crystalline samples, a reversible second-order phase transition from the α-phase (with soluble hydrogen) through a mixture of α- and β-phase into a pure β-phase was found. In amorphous samples, no transition was found. The saturation magnetization of the samples increases with hydrogenation and further increases upon hydrogen desorption. The increase of the Ni/Fe ratio in the TiFe1-xNi2 system is found to result in an increase of hydride cohesive energies and in the systematic shifting of the Fermi energy to lower values, in both pure intermetallics and appropriate hydrides. The hydrogen desorption temperature rises but the maximum amount of hydrogen absorbed under the same conditions decreases. Among the studied materials, TiFe0.8Ni0.2 was found to be the most promising composition for hydrogen storage.
Mechanochemical synthesis, elastomers and liquid crystals

Using quadrupole-perturbed nuclear magnetic resonance of $^{23}$Na, we monitored the chemical processes governing the mechanochemical synthesis of NaNbO$_3$. The results reveal the existence of a transitional amorphous carbonato complex with an atypical Nb-O bond. We successfully detected $^{14}$N quadrupole-perturbed nuclear magnetic resonance in photoisomerizable nematogen 7AB, in spite of extremely short spin-lattice relaxation times, typically about 10 us, which combined with a large quadrupole coupling constant normally inhibit the detection of resonance. In the specific case of 7AB, a relatively small and well-resolved $^{14}$N quadrupole doublet can nevertheless be detected, since the N-N bond exhibits reorientations about the long molecular axis at the angle close to the magic angle. Taking into account the differences in the temperature dependence of $^2$H and $^{14}$N doublet splittings, we also determined the temperature dependence of the molecular biaxiality. The temperature-concentration ($T$-$f$) phase diagram of the binary confined liquid crystal 7AB was also determined (Figure 10). The non-equilibrium concentration of cis-isomers, $f$, was controlled by illumination with UV light. The establishment of the equilibrium state with all trans-isomers was monitored in-situ via the quadrupole-perturbed nuclear magnetic resonance of $^2$H.

Ferroelectrics, hydrogen-bonded systems, pharmaceutical and biological substances

We investigated organic ferroelectrics, hydrogen bonds, pharmaceutical and biological substances, cocrystals and crystal polymorphs. Phase transitions in a metal-organic perovskite with an azetidinium cation, which exhibits giant polarizability, were investigated using differential scanning calorimetry (DSC) and $^1$H nuclear magnetic resonance (NMR) measurements. The DSC results indicated successive phase transitions at 254 and 299 K. The temperature dependence of the spin-lattice relaxation time $T_1$ determined by NMR indicated that the activation energy for cation ring-puckering motion was 25 kJ mol$^{-1}$ in phase I ($T > 299$ K).

The $^{17}$O NQR frequencies have been measured in cis-cyclobutane-1,2-dicarboxylic acid and the quadrupole coupling tensors have been determined at various temperatures. The temperature dependence of the $^{17}$O quadrupole coupling tensors at the $^{17}$O···H-O oxygen positions was analysed in the model of proton exchange and the energy differences of the two proton configurations obtained by this analysis agree with the values obtained from the O-H distances. The model shows that the population of an oxygen lone pair orbital is at this oxygen position reduced from 2 to approximately 1.3.

The stability of the antihypertensive drug nifedipine (NIF) has been studied in the solid state by $^1$H-$^{14}$N NQR double resonance (NQDR) and theoretically by the Density Functional Theory (DFT). The photoconversion of NIF to NO$-$NIF in the solid was found to be accompanied with the electron density redistribution at nitrogen sites (-NH$_2$ to –N= and -NO$_2$ to -NO) and proved to be successfully detected with the identification of photoproducts by $^1$H-$^{14}$N NQDR and DFT methods. A potential anti-leukemic and anti-cancer agent, 2-thiocytosine (2-tc), has been studied experimentally in the solid state by $^1$H-$^{14}$N NMR-NQR double resonance (NQDR) and theoretically by the quantum theory of atoms in molecules (QTAIM)/density functional theory (DFT). Eighteen resonance frequencies on $^{14}$N were detected at 180 K and assigned to particular nitrogen sites (-NH$_2$, -N= and -NH$-$) in 2-thiocytosine. This study demonstrates the advantages of combining NQDR and DFT to extract detailed information on the H-bonding properties of crystals with...
complex H-bonding networks. Solid-state properties were found to have a profound impact on the stabilities and reactivities of both compounds.

Nuclear quadrupole resonance (NQR) was used as a method for the characterization of cocrystals and crystal polymorphs. $^{14}\text{N}$ NQR spectra of several cocrystals of carbamazepine have been measured together with the $^{13}\text{N}$ NQR spectra of cocrystal formers. The results show that the $^{14}\text{N}$ NQR spectrum of a cocrystal and the $^{13}\text{N}$ NQR spectra of cocrystal formers differ well outside the experimental resolution. It is further described how the NQDr techniques, that have been used to measure the $^{14}\text{N}$ NQR frequencies, can be used to check the homogeneity of a polycrystalline sample and to monitor the stability of a metastable crystal polymorph.

Nitrogen atoms are present in a number of solid explosives and illicit substances. The nuclear quadrupole resonance (NQR) spectra and spin–lattice relaxation of the nitrogen atomic nucleus $^{14}\text{N}$ can be used to characterize these compounds and to distinguish between possible crystal polymorphs. After the characteristic $^{14}\text{N}$ NQR frequencies and spin–lattice relaxation rates in a compound are determined, NQR can be used to detect these compounds and, in the case of crystal polymorphs, also to determine the method of preparation. The $^{14}\text{N}$ NQR frequencies and spin–lattice relaxation rates are measured either by pulse NQR or by nuclear quadrupole double resonance (NQDr) based on magnetic field cycling.

II. Research programme “Physics of Soft Matter, Surfaces and Nanostructures”

The investigations of the research program “Physics of Soft Matter, Surfaces and Nanostructures” are focused on novel complex soft matter systems and surfaces with specific functional properties. We investigated in particular liquid-crystalline elastomers and dendrimers as novel multifunctional materials, nematic colloids, molecular motors, soft matter photonic crystals and novel synthetic or self-assembled micro- and nano-structures. The aim of the program is to understand the structural and dynamical properties of these systems, their interactions, their function at the molecular level, and self-assembly mechanisms in soft matter. The underlying idea is that it is possible to understand complex mechanisms, such as self-assembly, on a macroscopic level, using a simplified physical picture and models. In order to provide a comprehensive approach to the problem, the program combines both experimental and theoretical investigations, supported by modelling and simulations. Special emphasis is given to the possible electro-optic and medical applications.

Modelling of the laser imprinting of defects in nematics

We showed that using Laguerre-Gaussian optical beams, complex structures of typically even higher complexity can be induced in nematics. The role of the absorption - in the bulk or at the surfaces - is addressed, demonstrating complex local heating of the nematic material within the optical beams. Finally, the structures imprinted by complex optical beams can be good candidates for various further-tuned structures affected by confinement, complex surface anchoring profiles, chirality of nematic, and incorporation into nematic colloids. The work was published in Soft Matter.

Rewiring of nematic braids in chiral nematic colloids

We studied chiral colloidal dimers on the theoretical and experimental level. The influence of the chirality on the tangles in the formalism of tetrahedral rotations is of vital importance if the formalism is to be used to predict the possible structures. Systems with sufficiently complex boundary conditions can assume a large number of metastable configurations. Accurate prediction and the guided simulation of complex structures can accompany the experimental results for chiral defect systems induced optically, by colloidal inclusions, or by confinement. The work was published in Soft Matter.

Modelling of cholesteric droplets

We addressed systems of cholesteric liquid-crystal droplets, where the relation between the confinement via the spherical surface of the droplet and the chiral twisting of the liquid crystalline orientational order is specifically expressed. Multiple anisotropic optical profiles are demonstrated, emerging as a result of geometrical confinement.
Also, the authors show that changing the intrinsic twisting of the molecular optical axes induces remarkable changes in the droplet structure, modifying the optical and photonic properties of the droplets. The demonstrated approach could be used as a possible mechanism to envisage soft-matter optic and photonic elements in all-photonics circuits. The work was published in *Soft Matter*.

Shape-tuning the colloidal assemblies in nematics

Using numerical modelling, we demonstrate two-dimensional self-assembly of triangular, square, and pentagonal submicrometer-sized platelets in thin layers of nematic liquid crystals. Platelets are decorated with disclinations leading to effective elastic dipoles or quadrupoles. Colloidal assemblies of chains of such elastic dipoles into periodic lattices are formed via diverse rotational and translational shifts to minimize the distortions in the surrounding nematic medium. The work was published in *Soft Matter*.

Elastic anisotropy driven nematic shell restructuring

Confining a nematic liquid crystal to spherical shells with planar degenerate surfaces gives rise to various defect configurations with the total topological charge +2. In eccentric shells all four disclinations with winding number -1/2 are positioned in the thinner region to minimize their length. By chemically functionalizing these defects one could fabricate colloids with tunable valence. The elastic constant anisotropy, which is experimentally controlled by varying the temperature, leads to a gradual change of defect positions in a notably asymmetric way. On the other hand, when the eccentricity of the shells is changed, the defects increase their separation in a roughly symmetrical way. Controlling the directional-binding capabilities of shells provides a possible route towards the controlled self-assembly of colloids for optical and photonic applications. The research was performed in collaboration with the group in Montpellier.

Dimensional crossover in nano-confined liquid crystals

On decreasing a characteristic confinement length of confined thermotropic liquid crystals (LCs) the role of wetting-surface interactions is gaining in importance due to increasing surface-to-volume ratio. In particular, if noncritical surface interaction exhibits a linear dependence on the order parameter it can erase the phase transition at a critical confinement length. We were the first to demonstrate, theoretically and experimentally, that a different scenario might appear in nanoconfined LCs in the case of relatively weak wetting interactions. Namely, with a decreasing confinement scale the effective dimensionality of the system is reduced and consequently, the 1st-order phase transition into an orientationally ordered phase is, due to symmetry reasons, replaced by the 2nd-order phase transition. We realized experimentally weak wetting conditions by exploiting memory effects and using relatively flexible LC molecules (12CB). The results were published in *Soft Matter*.

Theoretical investigations of artificial swimmers.

We investigated the energetic efficiency of low Reynolds number swimmers driven by self-propulsion along their surface. An example of such swimmers are ciliated protozoa, but also artificial chemiphoretic swimmers. It turns out that the cost of propulsion is proportional to the square of the fluid velocity above the surface, integrated over the surface of the swimmer. We thus determined the swimmer shapes and their velocity distribution in a way that they achieve a given swimming velocity with minimum dissipation while keeping the volume constant. The result is surprising as the optimal shape can, depending on the allowed curvature, contain protrusions along the symmetry axis (Fig. 16 a). The calculated optimal swimmer shapes also show a high degree of similarity with various microorganisms found in nature (Fig. 16b). The work was published by A. Vilfan in *Phys. Rev. Lett*.

Vapour-trace detection of explosives using chemically functionalized COMB microsensors.

In collaboration with the Faculty of Electric Engineering and the Faculty of Chemistry and Chemical Technology of the University of Ljubljana we have developed and tested a miniature system for the detection of very small concentrations of vapours of various explosives in the atmosphere. The system is based on a very
sensitive microcircuit that uses planar COMB capacitors produced in CMOS technology. The vapour traces of explosives, which are always present in the vicinity of explosive devices, are selectively adsorbed on the electrodes of micro-capacitors that have been previously chemically functionalized with receptor molecules. This change in the capacity of the chemically functionalize capacitor is detected with the sensitivity in the range of an attofarad. We have succeeded in detecting 2 molecules of TNT in 10^14 molecules of the carrier gas N_2 (Figure 17).

Friction reduction via single MoS_2 “mama”-tubes and single MoS_2 fullerene-like particles

For the first time the coefficients of friction between a silicon AFM tip and a single MoS_2 nanotube or a single MoS_2 nano-onion were found to be much below the values obtained for a flat MoS_2 single crystal or graphite. We revealed a non-trivial dependency of the coefficient of friction on the interaction strength between the nanotube and the underlying substrate that is explained with the dissipation of energy and shear deformation. The MoS_2 nanotubes with a high interaction strength revealed up to four times larger coefficient of friction 0.08 than weakly supported tubes. The results explain the phenomena of the higher friction found for intra-crystalline slip than for inter-crystalline slip. This phenomenon, which is in contradiction with commonly accepted models, was published a quarter of century ago and remained without confirmation until now. We also evidenced that a rolling mechanism of MoS_2 fullerene-like nano-onions is indeed possible at low loads in accordance with recent predictions. The work was published Nanoscale Research Letters.

The addition of the MoS_2 nanotubes to the synthetic Polyalphaolefin (PAO) oil significantly improved the friction and wear behaviour in the boundary-lubrication conditions between AISI 52100/DIN 100Cr6 steel counterparts. The coefficient of friction was decreased by more than 2 times, while the wear was reduced by as much as 5-9 times. The use of nanotubes almost completely eliminated any abrasion or deformation of the surfaces in the studied time span. The investigation showed that the formation of a MoS_2 nanotubes-based tribofilm in the contact area was of key importance for the reduction of friction and wear.

MoS_2 nanotubes mediated polymer melt-processing for novel nano-composites materials

The MoS_2 nanotubes were introduced into an isotactic polypropylene (iPP) polymer matrix to generate novel nanocomposite materials through an advantageous melt-processing route. The incorporation of iNT-MoS_2 generated notable performance enhancements through reinforcement effects, highly efficient nucleation activity, and excellent lubricating activity in comparison with other nanoparticle fillers. The thermal stability of nanocomposites filled with 1 wt.% of iNT-MoS_2 was almost 60°C higher than that of neat iPP; the coefficient of friction decreased by 15% and wear by more than 50%.

Chemically synthetized field-effect transistor (FET)

We report the realization of FETs made with a chemically synthesized, layered 2D semiconductor crystal of WS_2. The 2D Schottky-barrier FETs demonstrated ambipolar behaviour and a high (∼10^5) on/off ratio at room temperature with current saturation. The behaviour was attributed to the presence of an energy bandgap in the 2D crystal material. The FETs show clear photoresponse to visible light. The promising electronic and optical characteristics of the devices combined with the layered 2D crystal flexibility make WS_2 attractive for future electronic and optical devices. This work was published in Applied Physics Letters.
III. Research programme “Experimental Biophysics of Complex Systems”

Within the program “Experimental Biophysics of Complex Systems” we explore processes and structures of various complex systems (from model systems to the structures in living cells, tissues and even small animals) including the effects of various bioactive molecules like toxins, drugs, etc., as well as of various materials like nanomaterials and medical materials on these systems. Our research is focused on the investigation of the structural properties of different membrane structures such as membrane domains, membrane proteins and glycosaccharide matrix as well as their interactions with various materials that enter into their native environment. Novel spectroscopic and micro-spectroscopic techniques contribute to the understanding of the organization of these supramolecular systems, complex cell and tissue responses as well as opening up new possibilities to design new medical materials, like scaffolds for tissue regeneration as one of the most relevant problems in the current aging population of developed countries. In addition, we focus on medical method optimization, like tumour treatment methods, magnetic resonance imaging and the mathematical modelling of thrombolysis, magnetic resonance microscopy in forestry, wood science and food processing as well as to restricted diffusion research.

One of the hottest topics in biophysics is the study of the interactions between novel materials and cells, especially from the bioactivity and bio-compatibility points of view, which we explore by applying novel micro-spectroscopies. We upgraded our system for fluorescence microscopy, which enables us to acquire fluorescence spectra from small volume elements of the sample and thus to detect physical changes in the local molecular environment of fluorescent probes, with new acquisition and analysis routines. By changing imaging sequence, introducing a spectral model, and implementing efficient computer simulations, we improved the spectral resolution and bleaching correction reliability. These advances – combined with custom designed environmentally sensitive probes – enabled us to observe phase transitions of single liposomes (Figure 23), to detect membrane microdomains, i.e., molecular motional patterns, and to determine the local pH in different parts of the cell. With the new system we can now use photobleaching of the probes to obtain new molecular information, which we showed when studying the influence of the B12 vitamin on cell-membrane resistance to external amphiphilic molecules. As a part of our cell-nanomaterial interaction research, we were investigating the rates and mechanisms of cells’ uptake of titanate nanoparticles. The system for micromanipulation was used for research on the dynamics and strength of cell attachment to macrostructured biomedical materials which are used as models for potential artificial tissue scaffolds.

In the area of the design and synthesis of probes (nitroxide, fluorophore and combination of both in the same molecule) in 2012 the focus was on the synthesis of fluorescent probes of the rhodamine type. Their fluorescence spectra are sensitive to changes of pH in the local environment. We have synthesized derivatives of rhodamine labelled mannose, showing high affinity for binding to DC-SIGN receptor on dendritic cells. Binding to the DC-SIGN receptor triggers the process of endocytosis. In this way we have prepared useful molecular tools for the study of cellular structures (e.g., lys-
was investigated by EPR and fluorescence spectroscopy. It was found that of EPR spectra we have found that the membranes are heterogeneous, but influence the fluidity of the archeosome membrane. By computer simulation become homogeneous at temperatures above 70°C.

The influence of OPP on the membrane fluidity of OPP-resistant MCF7, and OPP-sensitive MT3 breast-cancer cell lines, as well as the accumulation of spin labelled OPP in cells was investigated. The results were compared to those obtained on mouse fibroblast (L929) cell lines. OPP increases the membrane fluidity of all cell lines. However, irrespective of the finding that spin-labelled OPP accumulates better in the sensitive MT3 cells as in the less sensitive MCF7 cells, the changes in membrane fluidity are less pronounced in MT3. Our results show no correlation between the cell membrane fluidity, its changes under the influence of OPP and the sensitivity of cells to OPP. The only correlation we found was between OPP sensitivity and the cell growth rate.

In collaboration with the Biotechnical Faculty of Ljubljana the properties of a new class of liposomes prepared from archal lipids (archeosomes) was investigated by EPR and fluorescence spectroscopy. It was found that the pH of the growth medium in the range between pH6 and pH8 does not influence the fluidity of the archeosome membrane. By computer simulation of EPR spectra we have found that the membranes are heterogeneous, but become homogeneous at temperatures above 70°C.

In collaboration with the Veterinary Faculty of Ljubljana we introduced the EPR method with spin trap Fe(Detc)_2 to measure the production of a reactive nitric oxide radical (NO) in organs of live animals. We detected the formation of NO in organs of mice after a single oral gavage with live Escherichia coli. The measurements indicate an early systemic inflammatory response to the infection. Our investigations so far show EPR as a reliable and efficient method for the detection of NO radicals in living organisms.

One of our main activities is also the study of membrane structuring (Figure 24). In this respect it is important to note that different time and distance scales of methods can lead to very different conclusions regarding the stability of the heterogeneous structure of membranes. We are therefore trying to study observed phenomena and processes with complementary methods. This enables us to better understand the complex problems that we encounter. For example, beside the EPR method we have studied the interaction of cancerostatic OPP with lipid membranes also by attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR). Consequently, we were able to confirm the influence of the composition of membranes on the level of OPP interaction with membranes. We were also able to exclude the influence of spin probes used in EPR on the OPP action, while no molecular probes are required for ATR-FTIR. The second example is the application of ATR-FTIR to examine the influence of protonation on the dynamics of the transformation of molecular bonds during the transition of a fluorescent dye from a cyclic to an open structure.

With the help of molecular dynamics (MD), we calculated the difference in the rotational diffusion of spin labels attached to the peptide, and surrounded by water or membrane. These results are the key to improving the empirical approximations of side-chain conformational space modelling (CSM). Such estimates allow us to significantly reduce the computational time needed for determining the size of the side-chain conformational space. This also enables us to solve inverse problems – for example, the structural characterization of membrane proteins. We found that the diffusion of the spin label in the membrane is approximately 5 to 10 times slower, but surprisingly the size of the available conformational space is very similar to the size available in water. We also used MD to select the 17 most appropriate cysteine mutants of a very interesting peptide, the N-terminal part of β-defensin, with a different 3D structure in a membrane or water environment. Peptide synthesis is still relatively expensive; by using MD simulations we can estimate the minimum number of key mutants needed for structural characterization. The resulting structure

In the article “Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli” published in Thrombosis Research, we showed that the shape of platelet inclusions in the blood clot can also be influenced by the flow of blood in the area of the clot formation and not only by the biochemistry of the corresponding processes.
will be compared to the results of NMR and will highlight the benefits of our (CSM) method for the structural characterization of membrane proteins.

We confirmed that the coating of titanate nanomaterials on polyethylene terephthalate (PET) exhibits antimicrobial activity, even when exposed to ordinary fluorescent lamps. In comparison with conventional disinfection processes, such as chemical and steam cleaning, maintaining clean surfaces with the antimicrobial coatings is potentially much less demanding and does not leave behind harmful chemical residues. Given the encouraging results of the antimicrobial activity of titanate nanocoatings, we started to develop a prototype of air and waste-water cleaners.

We have shown that dimerization of factor Xa plays an important role in the process of blood clotting or coagulation, in collaboration with researchers from the University of North Carolina. Our results demonstrate that the dimerization site and factor Va-binding site are both located in the catalytic domain of factor Xa and that these sites are linked thermodynamically. We assume that the linkage between the dimer interface and factor Va-binding regions of factor Xa may have a physiological significance in blood coagulation. We speculate that factor Xa dimerization is a mechanism that limits prothrombinase formation when blood clotting is undesirable. We are investigating this possibility using model membranes.

Thrombolysis is a process in which the addition of specific reagents to the bloodstream can dissolve blood clots. So far, thrombolysis was in the literature dealt primarily as a biochemical process. However, in the last few years we have shown that mechanical forces on the flow of the blood clot are also very important for successful thrombolysis. Therefore, thrombolysis can also be regarded as a kind of corrosion-erosion process. In the past year we published two articles which present a model of thrombolysis as a corrosion-erosion process: “Analysis of blood clot degradation fragment sizes in relation to plasma flow velocity”.

Magnetic resonance imaging is a useful tool to show the heterogeneity of blood clots. With this method we can distinguish between areas that are predominantly composed of platelets, and are resistive to thrombolysis and areas that are predominantly composed of red blood cells and are more susceptible to thrombolysis. In the published article, we showed that the shape of the platelet inclusions in the blood clot can be explained by the flow of blood in the area of clot formation: “Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli. Thromb. res., 2012, vol. 129, issue 2, str. 158-163.”

Magnetic resonance imaging (MRI) was used to study water distribution and its mobility in the common bean during soaking at room temperature and cooking of pre-soaked and dry bean. To obtain the total water uptake, a combination of two MRI methods were used: a 3D RARE method that emphasizes the area where highly mobile (bulk) water is present and the signal of low mobile (bound) water is weak or even not observed and a 3D SPI method that emphasizes the area where water restricted in motion is present, but suppressing the bulk water signal owing to the short repetition time. It was shown that by the combination of the 3D SPI and the 3D RARE imaging techniques a complete insight into water distribution in the bean can be obtained and simultaneously tracing of mobile and bound water that penetrated into the bean seed is feasible.

Controlled drug delivery systems are widely used in the pharmaceutical industry because of their numerous advantages. For hydrophilic polymers, it is generally accepted that, once in contact with body fluids, they hydrate and swell, forming a gel layer that regulates the penetration of body fluids into the tablet and the dissolution of the incorporated drug. Therefore, the knowledge of the gel layer characteristics is of crucial importance for the use of controlled drug delivery systems. A combination of different MRI methods enables an accurate determination of the medium penetration into the tablet as well as hydrogel formation in situ. This approach has been used to determine the influence of the highly soluble incorporated drug in matrix tablets of xanthan on the kinetics.
of medium penetration and hydrogel formation. The influence of the drug was studied in media with different pH and ionic strengths. The impact of the drug on the hydrogel thickness was found to be dependent on the medium conditions. The drug does not change the hydrogel thickness in a water medium, whereas in acid medium the presence of the drug results in thinner hydrogel. The increased ionic strength in water medium also leads to the formation of the thinner hydrogel layer, while the effect of NaCl in HCl pH 1.2 medium being very small.

Magnetic resonance imaging allows monitoring of the distribution of electric current density in the conductive samples. By using current images in several different arrangements of electrodes, it is possible to determine the electrical conductivity of the sample and consequently also the electric field for a given electrode arrangement. This is of paramount importance in electroporation, which is a method in which by the use of high voltage the cell membrane is a tissue that is made temporarily permeable and therefore absorbs more drugs than normally, as for example anti-cancer drugs.

Magnetic resonance imaging is also very efficient in showing soft tissues in teeth, especially dental pulp (Figure 25). This method can be used to study anatomy or dental pulp or may even be used to detect early effects of dental caries on the pulp. Latter can be detected by ADC mapping of the pulp region.

Our research has been supported by a number of international projects financed by the European Union within the Sixth and Seventh Frameworks. It was also supported within the bilateral Slovenian – USA, Slovenian – German and Slovenian – Greek and other scientific cooperations. In 2012, we had cooperations with 108 partners from Slovenia and abroad. Among them

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field centre at the University Florida, Tallahassee, Florida, USA
- The ETH, Zürich, Switzerland
- The Ioffe Institute in St. Petersburg, Russia
- The University of Duisburg, the University of Mainz and the University of Saarbrucken in Germany
- The University of California, the University of Utah and the Liquid Crystal Institute, Kent, Ohio, USA
- National Institute for Research in Inorganic Materials, Tsukuba, Japan
- NCSR Demokritos, Greece
- Institut für Biophysik und Nanosystemforschung OAW, Graz, Austria
- Bioénergétique et Ingénierie des Protéines, CNRS Marseille, France
- Architecture et Fonction des Macromolécules Biologiques, CNRS Marseille, France
- The Max Delbruck Center for Molecular medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA
- The Mayo Clinic, Rochester, USA

made the above studies possible.

Some outstanding publications in 2012


Figure 24. Spin label in three different environments: vacuum, water and membrane as calculated in MD.

Figure 25. MRI image of a dental pulp in different stages of caries (lowest - ICDAS 0 to the maximum - ICDAS 6). Images on the left are T1-weighted and show the anatomy of the dental pulp, images on the right are corresponding ADC maps in which regions affected by caries appear purple, while healthy pulp is in pink.
Some outstanding publications in 2011


Awards and appointments

1. Primož Koželj: Prešern award of the Faculty of Mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Electrical, magnetic, and thermal properties of the δ-FeZn10 complex intermetallic phase,

2. Samo Kralj: Golden sign, Maribor, University of Maribor

3. Miha Škarabot, Igor Muševič: Luckhurst Samulski prize, Mainz, Liquid Crystals


5. Gregor Posnjak: Prešern award of the Faculty of Mathematics and Physics for Diploma thesis, Ljubljana, University of Ljubljana, Magnetic structure determination of one-dimensional antiferromagnet CuSe20S with neutron scattering


7. Uroš Tkalec: Glenn H. Brown Prize, Mainz, International Liquid Crystal Society

Organisation of conferences, congresses and meetings


2. 8th Physicists Conference in Basic Research, Rimske Toplice, Slovenia, 19. 10. 2012

Patent granted

1. Igor Muševič, Matjaž Humar, Spherical liquid crystal laser, SI23567 (A), Urad RS za intelektualno lastnino, 31.5.2012
INTERNATIONAL PROJECTS

1. NMR Spectrometer
   Korea Basic Science Institute
   Prof. Janez Dolinšek

2. MERCK - AFM investigations
   Merck KGaA
   Asst. Prof. Milka Skarabot

3. 7. FP - HIERARCHIC: Hierarchical assembly in controllable matrices; 215851, PITN-GA-2008-215851
   European Commission
   Prof. Igor Muševič

4. 7. FP - UNCOVER: Underwater coastal sea surveyor
   European Commission
   Prof. Robert Bilic

5. 7. FP - DIAGNO-RAIL: Combining innovative portable visual, acoustic, magnetic and NMR Methods with In-vivo chemical diagnostic tools for effective failure assessment and maintenance strategy of rail and subway systems
   European Commission
   Prof. Janez Dolinšek

6. 6. FP - LEMSUPER: Light element molecular superconductivity: An Interdisciplinary approach
   European Commission
   Prof. Denis Arčon

7. 7. FP - ENSSTM: Electron spin noise scanning tunneling microscopy
   European Commission
   Prof. Janez Dolinšek

8. 8. FP - NanoMag: Magnetic nanoparticles and thin films for spintronic applications and high performance permanent magnets
   European Commission
   Prof. Janez Dolinšek

9. Structure and mechanism of cytoplasmic dynein
   HFSP - International Human Frontier
   Asst. Prof. Andrej Vilač

10. COST MP1003: ESNAM - European scientific network for artificial muscles
    COST Office
    Prof. Boštjan Zalar

11. COST IC1101: Network for intermetallic compounds as catalysts for steam reforming of methanol
    COST Office
    Prof. Janez Dolinšek

12. NATO ARP 984477: Magnetic resonance detection of explosives and illicit materials, 2 - 7. 9. 2012, Turkey
    NATO
    Asst. Prof. Tomaz Apil

13. COST MP1203: Rational design of hybrid organic-inorganic interfaces: The next step towards advanced functional materials
    COST Office
    Dr. Polona Umak

14. HiEriMP Workshop 2012: Workshop on assembling of superstructures in soft matter
    Prof. Igor Muševič

15. Dielectric and electrocaloric properties of advanced relaxor dielectric polymer films and nanotubes
    Slovenian Research Agency
    Asst. Prof. Vid Bohar

16. Geometrically frustrated quantum magnetism
    Slovenian Research Agency
    Dr. Andrej Zorko

17. BI-FR/11-12-POTEUS-008: Novel states of matter induced by frustration in quantum magnets
    Slovenian Research Agency
    Dr. Polona Umak

18. Hydrogen storage in metal hydrides and nanomaterials
    Slovenian Research Agency
    Asst. Prof. Tomaz Apil

19. Factor Xa dimerisation and its role in prothrombinase complex formation and activity on membrane surfaces
    Slovenian Research Agency
    Dr. Marjeta Sentić

20. Synthesis, microscopy characterization and magneto resonance study of new functional nanomaterials
    Slovenian Research Agency
    Dr. Polona Umak

21. BI-FR/12-13-POTEUS-001: Unconventional ground states of quantum matter
    Slovenian Research Agency
    Dr. Martin Klanišek

22. Exotic electronic properties arising from geometrical symmetry
    Slovenian Research Agency
    Prof. Denis Arčon

RESEARCH PROGRAMS

1. Magnetic resonance and dielectric spectroscopy of „smart“ new materials
   Prof. Janez Dolinšek

2. Physics of soft matter, surfaces and nanostructures
   Prof. Slobodan Žumer

3. Experimental biophysics of complex systems
   Prof. Janez Stepnišek

R & D GRANTS AND CONTRACTS

1. Dentin evolution detected by spectroscopic means
   Prof. Janez Strancar

2. Novel ground states and quantum critical points in low-dimensional quantum spin systems
   Dr. Andrej Zorko

3. Use of nanoparticles as additives in lubricants and in tribology
   Prof. Maja Remškar

4. Optical microresonators based on liquid crystals
   Prof. Igor Muševič

5. New metallic materials for thermal storage of digital information
   Prof. Janez Dolinšek

6. Design, formulation and characterization of biomimetic nanocomposite systems for effective tissue regeneration
   Dr. Mojca Urtiča Mikač

7. Theory of the nematic nanodroplet and ordering of DNA, encapsulated in simple viruses
   Asst. Prof. Andrej Vilač

8. Collective and molecular dynamics of photoreactive liquid crystal elastomers
   Prof. Boštjan Zalar

9. Advanced ferroelectric polymeric and inorganic materials: Giant electrocaloric effect and transport properties
   Prof. Ždravko Kutnjak

10. Hydrogen storage in Zr-based metallic glasses
    Prof. Janez Dolinšek

11. New methods for the detection of N-nuclear quadruple resonance
    Asst. Prof. Tomaz Apil

12. Molecular motors
    Asst. Prof. Andrej Vilač

13. Superconductivity and magnetism in new iron-based superconductors
    Dr. Peter Jogič

14. Three dimensional assembling of colloidal structures in mesophases
    Prof. Slobodan Žumer

15. Hybrid nanomaterials for low-friction polymer composites and energy conversion
    Prof. Maja Remškar

16. Study of food processing and preparation by magnetic resonance imaging and spectroscopy methods
    Prof. Igor Šerša

17. Textured ceramic films for sensors and actuators
    Prof. Ždravko Kutnjak

    Dr. Polona Umak

19. Oligomers of amyloidogenic proteins from a to z: biophysical properties, structure, function and mutual interactions
    Asst. Prof. Milka Skarabot

20. Bionanotechnological processes of treatment of lignocellulosic materials
    Prof. Janez Strancar

21. Behaviour of dispersive systems under extreme thermo-mechanical loading
    Dr. Matej Pregelj

22. Eye Protection
    Dr. Janez Pirš

23. New materials for power conversion: Oxide semiconductor thermoelectrics
    Prof. Boštjan Zalar

24. A spectrometer for automatic 14N nuclear quadrupole resonance characterization of new substances
    Dr. Alan Gregorovič

25. TARANA: Targeting antimicrobial activity via micro/nano-structured surfaces for civil applications
    Prof. Janez Strancar

26. Nanomaterials and Scaffolds preparation and characterization
    Prof. Janez Strancar

27. CONFIRMER: Counterfeit pharmaceuticals interception using radiofrequency methods in realtime
    Asst. Prof. Tomaz Apil

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NEW CONTRACTS

1. A spectrometer for automatic 14N nuclear quadrupole resonance characterization of new substances
   Goreme Household Appliances, d. d.
   Dr. Alen Gregorovič

2. CONIFERME Counterfeit pharmaceuticals interception using radiofrequency methods in realtime
   Prof. Igor Muševič

VISITORS FROM ABROAD

3. Dr. Igor Govorovsky, Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine, 1. – 31. 3. 2012
4. Prof. Yshay Manassen, Department of Physics, Ben Gurion University, Beersheba, Israel, 19.–22. 2. 2012
5. Dr. Magdalena Wencza, Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland, 1.–31. 6. 2012
6. Prof. Iztok Pugliese, Department of Physics, Ben Gurion University, Beersheba, Israel, 19.–22. 2. 2012
8. Dr. Nikolaus Nölke, BASF, Heidelberg, Germany, 24.–27. 4. 2012

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55. Ilija Jonecek, B. Sc.
56. Andrej Kocan**
57. Primoz Kolesnik, B. Sc.
58. Andrej Krstic, B. Sc., left 01.12.12
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64. Jana Milevški, B. Sc.
65. Nikola Novak, B. Sc.
**BIBLIOGRAPHY**

**ORIGINAL SCIENTIFIC ARTICLE**


Peter Gottmann, Stefan Rembein, Carla Bittencourt, Polona Umeek, Xiaoxing Ke, Gustaaf Van Tendeloo, Christopher Paul Ewels, G. Schneider, "Nanoscopie spectroscopy with polarized X-rays by NEXAFS-TXM", Nat. Commun. (Print), vol. 6, no. 1, pp. 1-5, 2015.


**INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH**


**REVIEWED SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK**


**PATENT**

1. Igor Muševič, Matjaž Humar, Spherical liquid crystal laser, SI23567 (A), Urad RS za intelektualno lastnin o, 31.5.2012.

**MENTORING**


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